Quantum Critical Point of the XY Model and Condensation of Field-Induced Quasiparticles in Dimer Compounds

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The quantum critical point of the three-dimensional XY model in a symmetry-preserving field is investigated. The results of Monte Carlo simulations with the directed-loop algorithm show that the quantum critical behavior is characterized by the mean-field values of critical exponents. The system-size dependence of various quantities is compared to a simple field-theoretical argument that supports the mean-field scaling.

KEYWORDS: quantum spin system, Heisenberg model, quantum Monte Carlo, XY model, XXZ model, cluster algorithm, loop algorithm, worm algorithm, directed-loop algorithm

Recent developments of the high-field magnets and related experimental techniques make it possible to explore the magnetic phenomena revealed only by a strong magnetic field. A typical example is the dimer compounds such as $TlCuCl_3$,[1,2] $KCuCl_3$[3] and $BaCuSi_2O_6$.[4] These compounds consist of dimers each being an antiferromagnetically coupled pair of spins. Without a strong magnetic field, spins form singlet pairs and the compounds are magnetically inactive. It was suggested[5,6] that when a strong magnetic field is applied to such a dimer system, triplet excitations are induced and the system may exhibit a phase transition at a finite temperature. This phase transition can be most naturally interpreted[7,8] as a condensation transition of the excitations that behave as bosonic quasiparticles. Indeed, the results of the Hartree-Fock (HF) calculation[7] of the diluted Bose gas qualitatively agree with the experimental observations, such as the characteristic temperature dependence of the magnetization and the algebraic temperature dependence of the critical magnetic field. Results of another recent experiment[9] also identified the phase transition as the Bose-Einstein condensation (BEC). Even a quantitative agreement was obtained[4] recently for $BaCuSi_2O_6$ for which the temperature dependence of the experimentally measured specific heat agreed with the Monte Carlo simulation results of the effective hard-core boson model, which showed a clear 'lambda' peak. Thus, the nature of the transition as a condensation transition of the triplet excitations has been established beyond reasonable doubt.

However, an unsettling disagreement has been left unsolved, in estimates of the critical exponent that characterizes the temperature dependence of the critical magnetic field. The experiments and the theories both suggest the algebraic dependence, $H_c(T) - H_c(0) \propto T^{\phi}$. However, the experimental estimates of ϕ range from 1.7[1] to 2.0,[2] whereas the theoretical estimate (namely, the HF value) is $\phi = 1.5$.[7] A Monte Carlo simulation[10] was performed recently on the effective spin model for $TlCuCl_3$. A temperature dependent effective exponent $\phi(T)$ was defined such that it characterizes the $H_c - T$ curve in a certain finite temperature-range centered at T. The simulation result showed that $\phi(T)$ is greater than 1.5 but seems to approach 1.5 as the temperature is decreased. Moreover, the HF calculation was elaborated recently[11] based on a more realistic dispersion relation for bosons determined by experiments. While it is doomed to yield only mean-field values of critical exponents, which obviously differ from the correct ones for a finite-temperature BEC transition, it still provides a fairly good approximation for the value of the critical temperature. Therefore, these recent simulation and theoretical studies may be suggesting that the failure of the HF approximation in the finite-temperature critical phenomena does not necessarily mean the failure in the quantum critical phenomena. In particular, the mean-field value $\phi = 1.5$ may be the correct and exact value near the zero temperature. This statement, however, has not been made conclusive because of the uncontrollability of the approximation and/or the various limitations (such as the system size and the temperature range) in the Monte Carlo simulation.

In this letter, we present a simple theoretical argument, from which one can conclude that the mean-field values of the critical exponents are exact for the quantum critical point (QCP), i.e., $T = 0$, $H = H_c(0)$, and therefore the inaccuracy of the HF approximation is not the reason for the disagreement. To demonstrate the validity of the argument, we also show some results of a quantum Monte Carlo simulation on the three-dimensional XY model with a magnetic field.

We start with the model in which each spin (e.g., each Cu spin in $TlCuCl_3$) is treated explicitly:

$$\mathcal{H} = \sum_i \hat{J} \boldsymbol{s}_{i1} \cdot \boldsymbol{s}_{i2} + \sum_{(ij)} \sum_{\alpha,\beta} \hat{J}'_{i\alpha,j\beta} \boldsymbol{s}_{i\alpha} \cdot \boldsymbol{s}_{j\beta} - \sum_{i\alpha} \hat{H} s^z_{i\alpha}.$$

Here, $\hat{J} > 0$ is the antiferromagnetic coupling constant that binds a pair of spins, i the index of the dimer and $\boldsymbol{s}_{i1}$ and $\boldsymbol{s}_{i2}$ the two spins that form the pair i. The lattice structure and the magnitude of the coupling constants depend on the compound. In the case of $TlCuCl_3$,[1] for example, the lattice is composed of double chains of spins (i.e., two-leg ladders) with relatively weak interlad-

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der couplings. The dominant couplings are theose corresponding to rungs of the ladder, which are represented by $\hat{J}$ above. Below, we assume that the interdimer couplings $\hat{J}'_{i\alpha,j\beta}$ are much smaller (in magnitude) than $\hat{J}$, and that the lattice is three-dimensional. Real materials, such as $TlCuCl_3$, are often strongly anisotropic. The spatial anisotropy is, however, irrelevant in the present letter since we focus on the critical properties, in particular, the critical properties near $T = 0$, where the three-dimensionality manifests itself.

Following Tachiki and Yamada,[5,6] we neglect the two of the triplet states that are not favored by the magnetic field. The remaining two states, the triplet state that is favored by the magnetic field and the singlet state, are regarded as the up and down states, respectively, of an effective $S = 1/2$ spin. The resulting Hamiltonian in terms of the effective spin $\boldsymbol{S}_i$ is[5,6]

$$\mathcal{H} = \sum_{(ij)} \tilde{J}_{ij} \left(S_i^x S_j^x + S_i^y S_j^y + \frac{1}{2} S_i^z S_j^z \right) - \sum_i \tilde{H}_i S_i^z, \quad (1)$$

where $\tilde{J}_{ij}$ and $\tilde{H}_i$ can be expressed as simple linear combinations of $\hat{J}$, $\hat{H}$ and $\hat{J}'_{i\alpha,j\beta}$. We here assume that the effective Hamiltonian is translationally invariant and non-frustrated. The experimental estimations of the lattice structure and the coupling constants suggest that these assumptions are valid, at least approximately, for several compounds such as $TlCuCl_3$[12] and $BaCuSi_2O_6$.[13]

Thus, we have arrived at the uniform $S = 1/2$ XXZ model in three dimensions with a spatial anisotropy and an easy-plane spin anisotropy. The common belief is that the spatial anisotropy does not affect the critical properties of the model both at the finite temperature transition and the QCP. In addition, the S^z-S^z term can be dropped without affecting the critical properties, since it does not change the type of spin anisotropy. Therefore, we can further simplify the model without changing the critical properties:

$$\mathcal{H} = -J \sum_{(ij)} \left(S_i^x S_j^x + S_i^y S_j^y \right) - H \sum_i S_i^z, \quad (2)$$

i.e., the XY model Hamiltonian. The sign of the coupling constant J can be switched by changing the spin representation bases. Therefore, we assume $J > 0$ and $H > 0$ without loss of generality in what follows.

If we consider the effective Hamiltonian as the sum of pair Hamiltonians H_{ij}, it is straightforward to show that the state in which the two spins S_i and S_j are aligned with the magnetic field is the unique ground state of H_{ij} when $H > dJ$. Therefore, the state with all spins pointed up is the unique ground state of the entire system for $H > dJ$. On the other hand, it can also be shown easily that mixing with one-magnon states decreases the energy of the all-up state when $H < dJ$. Therefore, for the present system, the quantum critical point is located exactly at $H = dJ$.

While the Hamiltonian (2) is the one that we simulate with the quantum Monte Carlo method, we can further reform it by using the bosonic representation $S_i^+ = b_i^\dagger$, $S_i^- = b_i$, and $S_i^z = \hat{n}_i - \frac{1}{2}$ with the constraint

$$\hat{n}_i \equiv b_i^\dagger b_i = 0, 1. \quad (3)$$

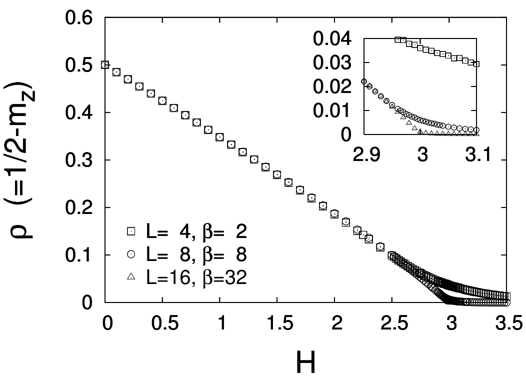

Fig. 1. Field dependence of magnetization $\rho \equiv \frac{1}{2} - \langle S_z \rangle$. The three curves correspond to different system sizes, while the 'scaled' temperature L^2/β is fixed to be 8. The inset is the close-up view of the quantum critical region.

Then we obtain

$$\mathcal{H} = -t \sum_{(ij)} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) - \mu \sum_i \hat{n}_i + \Lambda \sum_i \hat{n}_i(\hat{n}_i - 1), \quad (4)$$

with new parameters t and μ corresponding to the old ones as $t \sim J/2$ and $\mu \sim H$. The Λ-term imposes the condition (3), approximately.

Generally, the replacement of the original 'hard' constraint by a 'soft' constraint may affect the critical properties around the QCP. In the present case, however, we consider that this modification does not change the essential properties because the typical occupation number is zero or much smaller than unity near the QCP even in the soft-core case, while the difference between the hard and soft constraints manifests itself only for the states of which $n_i \geq 2$.

In the following few paragraphs, we present the results obtained earlier[14,15] for the Bose gas that can be found also in textbooks.[16] We reproduce them here since it is convenient to have explicit formulas in the form directly comparable with the present Monte Carlo results. (In particular, explicit formulas for the system-size dependence are hardly found in the literature.) First, the continuous field theory for model (4) is characterized by the action

$$\begin{aligned} S &= \int d\boldsymbol{x} \int d\tau \, \left(\psi^* \frac{\partial \psi}{\partial \tau} + |\nabla \psi|^2 \right. \\ &\qquad \left. - h \, \mathrm{Re}\, \psi - r\, |\psi|^2 + u\, |\psi|^4 \right). \end{aligned} \quad (5)$$

The parameter r depends on μ as $r \propto \mu - \mu_c$ near the QCP, and the symmetry-breaking field h, which does not correspond to the original magnetic field, is included for a technical purpose. From a simple dimensional analysis, the effect of the scale transformation up to the scale b turns out to be the following:

$$\beta \to \tilde{\beta} \equiv \beta b^{-2}, \; L \to \tilde{L} \equiv L b^{-1}, \; \psi \to \tilde{\psi} \equiv \psi b^{\frac{d}{2}},$$
$$h \to \tilde{h} \equiv h b^{2+\frac{d}{2}}, \; r \to \tilde{r} \equiv r b^2, \; u \to \tilde{u} \equiv u b^{2-d},$$

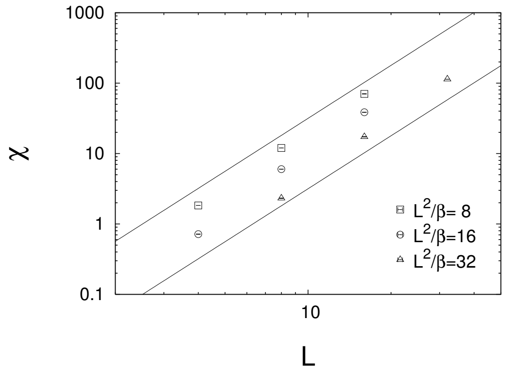

Fig. 2. Size dependence of susceptibility at quantum critical point, $H = 3J$. Three values of the scaled inverse temperature, $\beta/L^2 = 8, 16$ and 32, are examined. The solid lines indicate the slope of $\chi \propto L^{2.5}$.

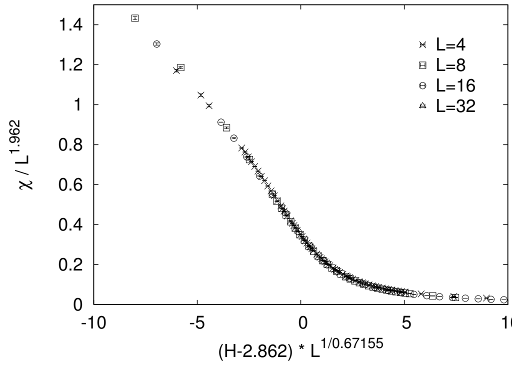

Fig. 3. Finite size scaling plot of susceptibility at $\beta = 4J$. The critical exponents used here are taken from the results of the classical XY model.[17]

where L is the system size. Hence, the upper critical dimension d_c is equal to 2.[14] For three dimensions, therefore, we should expect a mean-field-type scaling.

Because of the dangerous irrelevant parameter u, the usual procedure of the finite size scaling, i.e., rescaling the coordinate and the abscissa by size-dependent factors, does not work. We first define $\Phi(h, r, u, \beta, L)$ as the singular part of $-\log Z(h, r, u, \beta, L)$. We assume that Φ has the property $\Phi(h, r, u, \beta, L) = \Phi(\tilde{h}, \tilde{r}, \tilde{u}, \tilde{\beta}, \tilde{L})$ for an arbitrary b. With this expression, we first consider the particle density ρ, which corresponds, in the original model, to the deviation of the magnetization (parallel to the magnetic field) from its saturation value. The particle density is related to the magnetization perpendicular to the field, which we denote as m, by $\rho \sim m^2 \sim |\psi|^2$. Then we have

$$\begin{aligned} m(r,u) &\equiv \lim_{h\to 0}\lim_{L\to\infty}\lim_{\beta\to\infty} L^{-d}\beta^{-1}\frac{\partial \Phi}{\partial h} \\ &= b^{-\frac{d}{2}}\tilde{m}(\tilde{r},\tilde{u}), \end{aligned}$$

where $\tilde{m}(\tilde{r},\tilde{u})$ is the magnetization of the renormalized system. When the system is renormalized up to the point where the correlation length is $O(1)$, we can neglect fluctuations and apply the mean-field-type calculation without a serious error in estimating $\tilde{m}$, which yields

$$\tilde{m}(\tilde{r},\tilde{u}) \sim \sqrt{\frac{\tilde{r}}{\tilde{u}}} = \sqrt{\frac{r}{u}}\, b^{\frac{d}{2}}$$

for sufficiently large b. Thus, we arrive at[14]

$$\rho \propto r \propto |H - H_c| \quad (T = 0). \tag{6}$$

Similarly, we can obtain the scaling form of the susceptibility (of the spin components parpendicular to the magnetic field) at $r = 0$:

$$\begin{aligned} \chi(u,\beta,L) &\equiv \lim_{h\to 0}\lim_{r\to 0}\int d\boldsymbol{x}\int_0^\beta d\tau\ \langle\psi^*(x,\tau)\psi(0,0)\rangle \\ &\propto b^2\tilde{\chi}(\tilde{u},\tilde{\beta},\tilde{L}). \end{aligned}$$

For sufficiently large b, we have

$$\tilde{\chi}(\tilde{u},\tilde{\beta},\tilde{L}) \sim \sqrt{\frac{\tilde{\beta}}{\tilde{u}}} \sim \sqrt{\frac{\beta}{u}}\, b^{\frac{d}{2}-1},$$

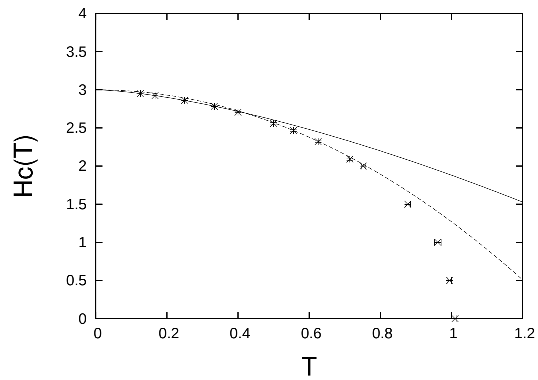

Fig. 4. Critical field as a function of temperature. The solid curve corresponds to $\phi = 1.5$, whereas the dashed curve $\phi = 2.0$.

where L is assumed to be larger than b. Therefore, the asymptotic system size dependence of the critical susceptibility for a fixed value of the scaled inverse temperature $\beta' \equiv \beta/L^2$ is

$$\chi(u, \beta' L^2, L) \propto L^{1+\frac{d}{2}}. \tag{7}$$

Finally, we consider the temperature dependence of the critical magnetic field. When $d > 2$, we can make $\tilde{u}$ small by choosing large b so that the perturbation theory in $\tilde{u}$ is nearly exact for the renormalized system. The perturbation theory indicates that Φ for the renormalized system has a singularity when the condition[16] $\tilde{r} = \tilde{r}_c \equiv A\tilde{u}/\tilde{\beta}^{d/2}$ is satisfied with A being a numerical constant. This means that in terms of the bare coupling constants, the singularity occurs when[14]

$$H_c(T) - H_c(0) \propto T^{d/2}.$$

We now present the results of our Monte Carlo simulation for spin Hamiltonian (2) on a simple cubic lattice and compare them with the theoretical predictions. The simulation method employed here is based on the directed-loop algorithm[18] for which a review can be found in a recent article.[19] The system sizes that we explored range from $L = 4$ to $L = 32$ and the temperatures from $\beta = 0.5$ to $\beta = 32$ (for $L = 32$).

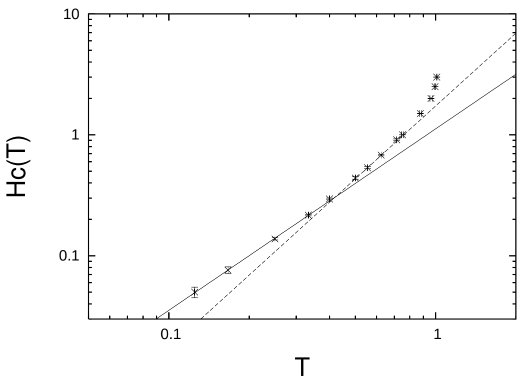

Fig. 5. Logarithmic plot of critical field against temperature. The two straight lines correspond to $\phi = 1.5$ (solid) and $\phi = 2.0$ (dashed). In the intermediate temperature region, $\phi = 2.0$ seems to fit the data well, while in the low-temperature region, the correct slope $\phi = 1.5$ yields a better fitting.

Figure 1 shows the magnetic field dependence of the deviation of the longitudinal magnetization from its saturation value. In the bosonic language, this is the particle density which is a function of chemical potential. Results are shown only for three system sizes $L = 4, 8$ and 16 with fixed 'scaled' temperature, $L^2/\beta = 8$. As can be seen in the figure, the system size dependence remains only in the vicinity of the quantum critical point. The inset shows the magnified view of the critical region. The linear field dependence (6) can be clearly observed in this inset.

Next, we show the susceptibility of the perpendicular components of spins. This is defined as $\chi \equiv \sum_{\boldsymbol{r}} \int_0^\beta d\tau \langle S^x(\boldsymbol{r}, \tau) S^x(\boldsymbol{0}, 0)\rangle$ for model (2). In Fig. 2, the system size dependence of the susceptibility at the critical point $H = 3J$ is shown. Three different values of the scaled temperature L^2/β are chosen. For each value of the scaled temperature, the asymptotic size dependence is well fitted by the straight line with the slope 2.5, in agreement with (7). Thus the universality class of the QCP is identified as the mean field type.

In order to obtain the phase diagram in the $H - T$ plane, we carry out the finite-size scaling of the susceptibility with a fixed magnetic field or a fixed temperature. As an example, a finite-size-scaling plot is shown for $\beta J = 4$ in Fig. 3. The data can be scaled nicely with the critical exponents estimated for the classical XY model, namely, $\nu = 0.67155(27)$ and $\eta = 0.0380(4)$.[17] The value of the critical field is the only free parameter determined by the present data, and the best plot is obtained for $H_c(T = 4J) = 2.862$. In this manner, we estimated the critical field (temperature) at various temperatures (fields).

In Fig. 4, two curves are plotted for comparison. The solid curve represents the mean-field critical exponent, $\phi = 1.5$, whereas the dashed curve represents the previous estimate[2] based on an experiment on $TlCuCl_3$, $\phi = 2.0$. At a first glance, it seems that the curve with $\phi = 2.0$ fits the data better than that with $\phi = 1.5$. However, when the logarithmic scale is used, as we do in Fig. 5, it is rather clear that $\phi = 2.0$ explains only a transient behavior, and the correct asymptotic value of the exponent is $\phi = 1.5$.

To summarize, we have argued that the mean-field exponents should be correct and exact for the quantum critical point of the XY model in three dimensions, and our numerical simulations demonstrated that it is indeed the case beyond reasonable doubt. Therefore, we can at least exclude the inaccuracy of the Hartree-Fock approximation as the source of the discrepancy between the theoretical and experimental results. We have also found that there is a relatively large intermediate temperature region where a transient behavior can be well described by the effective exponent $\phi \sim 2$. While there could be some other possibilities that may truly change the critical behavior from the mean field type to something else, such as a presence of Dzyaloshinsky-Moria interactions, the present results suggest that it is possible to explain the discrepancy between the theoretical and experimental results only by taking into account the transient behavior and that the quantum critical behavior driven by the magnetic field can be correctly described by the XY model (or the diluted Bose gas fixed point) which yields the mean-field exponents.

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